Nutritional metabolomics

object specific lipoprotein profiles and fat boosting

Mikkelsen, Mette Skau; Savorani, Francesco; Rasmussen, Morten Arendt; Jespersen, Birthe P Møller; Kristensen, Mette; Engelsen, Søren Balling

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– Object specific lipoprotein profiles and fat boosting

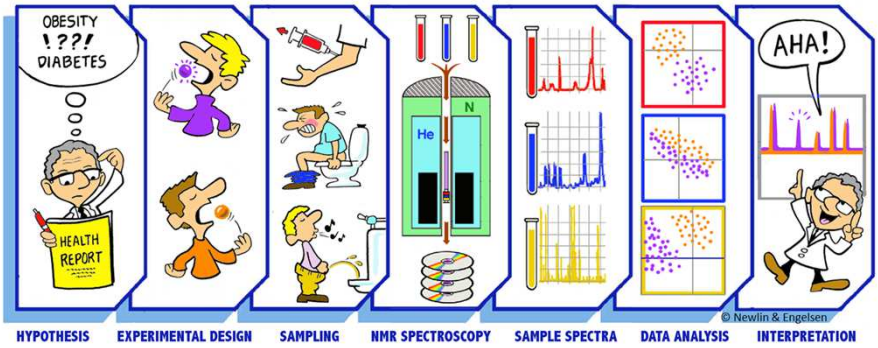
UNIVERSITY OF COPENHAGEN
FACULTY OF SCIENCE
DEPARTMENT OF FOOD SCIENCE

Mette Skau Mikkelsen [a†], Francesco Savorani [a†], Morten A. Rasmussen [a], Birthe M. Jespersen [a], Mette Kristensen [b] and Søren B. Engelsen [a]

[a] Dept. Food Science - Quality & Technology, [b] Dept. Nutrition, Exercise and Sports
[†] Presenting author. E-mail: Mette - skau@life.ku.dk; Francesco – frsa@life.ku.dk

Nutritional metabolomics

Nutritional metabolomics seeks to relate the intake of a particular dietary component to specific metabolic fingerprints.



The workflow of a nutritional metabolomics study involves hypothesis, experimental design, sampling of biofluids, the analytical platform, the sample spectra, data preprocessing, the multivariate data analysis and last but not least the biological interpretation[1].

Motivation

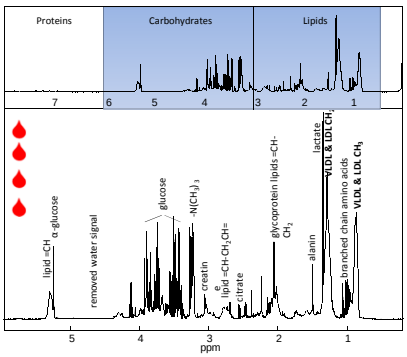
By using nutritional metabolomics techniques, it may be possible to detect additional nutritional responses to those found with the traditional biomarkers[1].

In this study, NMR spectroscopy in combination with multivariate data analysis is applied to investigate the full blood metabolic effects of daily supplementation of mixed linkage β-glucans from oat and barley[2, 3].

Both targeted and explorative metabolomics approaches are used.

^{1}H NMR spectroscopy

Proton nuclear magnetic resonance profiling of blood plasma reveals hundreds of small metabolites.



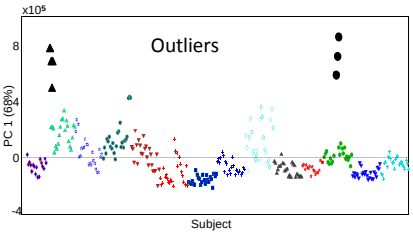
Top An average ^{1}H NMR Carr-Purcell Meiboom-Gill (cpmg) spectrum of human plasma (0-8 ppm) with spectral regions dominated by proteins, carbohydrates and lipids, respectively. **Bottom** Enlargement of carbohydrate and lipid regions (0.5-6 ppm).

Assignment of the spectra is made according to previous investigations[4] with the most important resonances for this study being the broad signals from the CH_2 and CH_3 protons in the lipoproteins (VLDL and LDL) at 0.9 and 1.3 ppm.

Multivariate data analysis

The complexity of metabolomics data makes interpretation complicated.

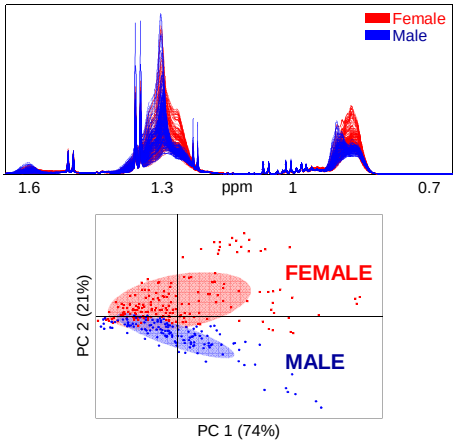
Multivariate data analysis can decompose data into simpler and more interpretable structures.



Principal component analysis (PCA) on plasma NMR spectra demonstrate that the main variance among samples is due to subject specific metabolomes.

Lipoprotein profiles

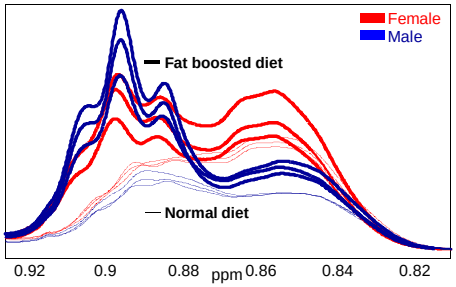
The second most influential variation in the data is due to gender and characteristic lipoprotein profiles are found for male and female samples.



Top Male and female plasma NMR profiles of the lipoprotein region (0.7-1.6 ppm). **Bottom** Score plot from PCA on all mean centered NMR spectra (0-8 ppm).

Fat boosting

Outlier samples caused by high fat diets show extreme lipoprotein signals as compared to normal samples.



NNR lineplot of the 0.9 ppm lipoprotein peaks for fat boosted outlier and normal samples.

The lipoprotein landscape is significantly sharpened by fat booting.

Conclusions

No significant blood metabolic exposure and effect markers were identified for intake of β-glucans from oat and barley as studied by targeted metabolomics.

Explorative metabolomics revealed the existence of subject unique lipoprotein profiles, which especially are dependent on gender and diet.

This leaves a potential for improvement of design in future nutritional metabolomics studies

References [1]Savorani, F et al. (2013), Food Res Int, *in press*; [2]Mikkelsen, MS et al. (2013), Food Chem, 136, 130-136; [3]Ibrügger, S et al. *(submitted)*, J Nutr; [4]Nicholson, JK et al. (1995), Anal Chem, 67, 793-811